

# Reading charge transport from spin dynamics on the surface of topological insulator

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Resolving the conductance of the topological surface states (TSSs) from the bulk contribution has been a great challenge for studying the transport property of topological insulators. By developing a non-perturbative diffusion equation that describes fully the spin-charge dynamics in the strong spin-orbit coupling regime, we present a proposal to read the charge transport information of TSSs from its spin dynamics which can be isolated from the bulk contribution by time-resolved second harmonic generation pump-probe measurement. We demonstrate the qualitatively different Dyakonov-Perel spin relaxation behavior between the TSSs and the two-dimensional spin-orbit coupling electron gas. The decay time of both in-plane and out-of-plane spin polarization is naturally proved to be identical to the charge transport time. The out-of-plane spin dynamics is shown to be in the experimentally reachable regime of the femtosecond pump probe spectroscopy and thereby we suggest experiments to detect the charge transport property of the TSSs from their unique spin dynamics.

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Topological insulators (TIs) are a class of time-reversal invariant matter<sup>1,2</sup>. Recently, both theory<sup>3-5</sup> and experiments<sup>6-12</sup> focus on the transport property of the TIs which have spin-momentum locking surface states. The helical topological surface states (TSSs) break the Fermi doubling and have very strong spin-orbit coupling (SOC) which gives their unique charge and spin transport properties<sup>13,14</sup>. However, in most TIs the bulk states also contribute the conductance, which makes it a great challenge to extract the transport properties of the TSSs, such as mobility, from the experimental data<sup>6,7</sup>. On the other hand, the spin polarization of the TSSs has been detected by the time-resolved second harmonic generation pump-probe measurement which can separate the surface response from the bulk<sup>8,9</sup>. This has not been possible until now because the complete spin dynamical theory of TSS is still absent due to the strong SOC of TSSs which can not be treated perturbatively as it is usually done in the traditional diffusive equation.

Here, we developed a non-perturbative spin dynamic theory to fully capture the spin dynamics of the TSSs which reveal the qualitative difference to that in other SOC 2DEGs such as GaAs quantum well<sup>15-17</sup>. The spin polarization along x,y,z direction are decoupled to each other even though the TSSs have strong SOC. The decay time of both in-plane and out-of-plane spin polarization is predicted to be exactly equal to the charge transport time,  $\tau_{tr}$ , instead of being proportional to the inverse of  $\Omega_{so}^2\tau_p$ , which is the commonly label Dyakonov-Perel (DP) mechanism. Here  $\Omega_{so}$  is the SOC frequency and  $\tau_p$  is the momentum scattering time. We estimate the time evolution of the out-of-plane spin dynamics which we show to be in the experimentally reachable regime of the femtosecond pump probe spectroscopy<sup>9</sup>. Because the surface spin dynamics can be isolated from the bulk contribution by recent second harmonic pump probe measurement<sup>8,9</sup>, we propose to read charge transport property of TSSs

from the spin by the pump probe measurement.

*Non-perturbative spin-charge dynamic equation on the surface of TI* - We assume that the low energy TSS has the Dirac-like Hamiltonian plus nonmagnetic short range disorder potential<sup>1,2</sup>

$$\hat{H} = v(\mathbf{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + V_0 \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \sigma_0, \quad (1)$$

where  $v$  is the constant velocity,  $\mathbf{z}$  is the unit vector perpendicular to the surface of TI,  $\mathbf{k}$  is the wave vector of the electron, and  $\sigma_0$  is  $2 \times 2$  identical matrix. Here we assume  $\hbar = 1$  and consider only spin independent scattering. The velocity operator has the form

$$\hat{\mathbf{V}} = \frac{\partial \hat{H}}{\partial \mathbf{k}} = v \mathbf{z} \times \boldsymbol{\sigma}, \quad (2)$$

and is proportional to the in-plane spin polarization perpendicular to the velocity direction.

The dynamics of the spin-charge polarization, as a non-equilibrium process, can be described by quantum Boltzmann equation<sup>18,19</sup>

$$\partial_t \hat{g} + \nabla_{\mathbf{R}} \cdot \left\{ \frac{1}{2} \hat{\mathbf{V}}, \hat{g} \right\} + i[\hat{H}_0, \hat{g}] + \frac{\hat{g}}{\tau_p} = \frac{\hat{\rho}}{\tau_p}, \quad (3)$$

where  $\hat{H}_0(\mathbf{k}) = v(\mathbf{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k}$  and

$$\hat{g}(\mathbf{e}_{\mathbf{k}}, \mathbf{R}, t) = - \int N(\epsilon_{\mathbf{k}}) \frac{dE d\epsilon_{\mathbf{k}}}{2\pi i} \hat{G}_{\mathbf{k},E}^K(\mathbf{R}, t), \quad (4)$$

is the angular distribution function<sup>20</sup>,  $\hat{G}^K$  is the  $2 \times 2$  matrix of spin- $\frac{1}{2}$  Keldysh Green's function,  $\mathbf{k}_{\mathbf{f}}$  is the Fermi wave length,

$$\hat{\rho}(\mathbf{R}, t) = \int \frac{d\theta}{2\pi} \hat{g}(\mathbf{k}_{\mathbf{f}}, \mathbf{R}, t) \quad (5)$$

is the density matrix,  $\tau_p$  is the momentum scattering time at Fermi surface,  $N(\epsilon_{\mathbf{k}})$  is the density of states,  $n_i$  is the 2D density of the nonmagnetic impurities and  $\theta$  is

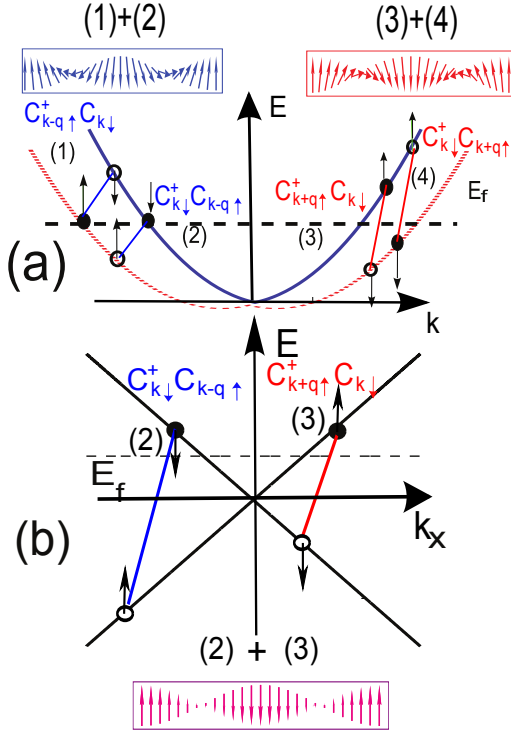


FIG. 1. (a) Spin polarization configure at  $k_y = 0$  channel in 2DEG. The solid(hollow) circle means creating(annihilating) an electron into the system which is corresponding to  $C^\dagger(C)$  operator. The clockwise SHM is constructed by  $\sum_k c_{k+q,\uparrow}^\dagger c_{k,\downarrow} + c_{k,\downarrow}^\dagger c_{k+q,\uparrow}$  (the red creation and annihilation operators) and the counter-clockwise SHM is constructed by  $\sum_k c_{k-q,\uparrow}^\dagger c_{k,\downarrow} + c_{k,\downarrow}^\dagger c_{k-q,\uparrow}$  (the blue creation and annihilation operators). Here  $\uparrow(\downarrow)$  as the subscripts indicates spin along  $+( - )$  y direction. The collective spin polarization plot in the rectangle boxes is in  $x - z$  plane. (b) Spin polarization configure at  $k_y = 0$  channel on the surface of TI. Because there is only one spin sub-band on the Fermi surface, the collective spin polarization arises from the summation of the half clockwise SHM and half counter-clockwise.

the angel between  $\mathbf{k}_f$  and the  $x$ -axis. Eq. A9 contains both commutation and anti-commutation relation of  $\hat{g}$ ,  $\hat{H}$ , etc. and can only be solved perturbatively. However the difficulty of obtaining the spin dynamics equation in the strong SOC regime lies on the fact that the spin precession angle  $2vk_f\tau_p$ , is too large to be treated perturbatively. This fact makes it difficult to apply Eq. A9 directly to the strong SOC regime. To circumvent this problem, we multiply  $\sigma_j$  where  $j = 0, x, y, z$  on both sides of Eq. A9 and calculate the trace. Using the fact that  $\text{Tr}(\sigma_j\sigma_k)/2 = \delta_{jk}$ , the quantum Boltzmann equation can be written in the classical spin-charge 4D space after integrating out  $E$  as<sup>19</sup>

$$\hat{K}_{jk}g_k = i\rho_j, \quad (6)$$

where  $g_j(\rho_j) = \text{Tr}[\hat{g}(\hat{\rho})\sigma_j/2]$  (the explicit form of  $\hat{K}$  is shown in the supplementary material). Here, we abandon the idea of gradient expansion in terms of  $\Omega\tau_p$  and

derive the spin-charge diffusion equation by simply multiplying  $K^{-1}$  on both sides of Eq.(A11) and integrating out the angle  $\theta$ . To simplify our discussion, we assume the uniform spin polarization along  $y$  direction, say  $\partial_y\hat{\rho} = 0$ . In this case, using the relation Eq.(A8), we obtain the non-perturbative spin-charge dynamic equation

$$\rho_j = \hat{D}_{jk}\rho_k, \quad (7)$$

where  $\hat{D} = \int \frac{d\theta}{2\pi} \hat{K}^{-1}$  and  $\hat{K}^{-1}$  has a complicated but analytically and numerically tractable form shown in the online supplementary material.

Eq. (A13) is a generalized spin diffusion equation and valid from the weak to the strong SOC regime. For the spin-momentum locked states, we have found that the spin polarizations along  $x$ ,  $y$  and  $z$  direction are completely decoupled even though the TSSs have very strong SOC. As a result, spin helical modes (SHMs) are absent on the surface of TI. The absence of SHM is due to the fact that for the TSSs there is only one spin degree of freedom on the Fermi surface. For an intuitive understanding of this fact, in Fig. 1, we schematically show that at the  $k_y = 0$  channel, the spin polarization modes of both 2DEG and the TSSs. For the spin polarization of the 2DEG shown in Fig. 1(a), there are two spin sub-bands on the Fermi surface which allow two SHMs with different two relaxation times<sup>16,21,22</sup>. In Fig. 1(b), because the non-equilibrium state is around the Fermi surface and  $E_f \gg kT$ , the spin sub-band below the Dirac point is still completely filled. Accordingly, at the  $k_y = 0$  channel the terms such as  $\sum_{k>0} C_{k,\downarrow}^\dagger C_{k+q,\uparrow}$  and  $\sum_{k<0} C_{k-q,\uparrow}^\dagger C_{k,\downarrow}$ , which add electrons to the spin sub-band below the Dirac point and thereby will not contribute to spin polarization. Here  $\uparrow(\downarrow)$  as the subscript of the creation or annihilation operator indicates spin along  $+( - )$  y direction. Therefore, the non-equilibrium spin polarization of TSSs around Fermi surface has only a  $z$ -component which is built from half clockwise terms containing  $\sum_{k>0} C_{k+q,\uparrow}^\dagger C_{k,\downarrow}$  and half counter-clockwise terms containing  $\sum_{k<0} C_{k,\downarrow}^\dagger C_{k-q,\uparrow}$ . The detailed discussion is presented in the online supplementary material.

*In plane spin dynamics along x direction.*- The spin polarization is completely decoupled for the spin polarization along  $x$ -direction. Its non-perturbative dynamic equation determining its complex frequency takes the form

$$1 - \frac{\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2} \sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \tilde{\Omega}_{so}^2}}{\tilde{\Delta}_x^2 \sqrt{\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2}} + \frac{\tilde{\Omega}}{\tilde{\Delta}_x^2} = 0, \quad (8)$$

where  $l$  is the mean free path,  $\tilde{\Omega} = 1 - i\omega\tau_p$ ,  $\tilde{\Omega}_{so} = 2vk_f\tau_p$  and  $\tilde{\Delta}_{x(y)} = lq_{x(y)}$ . Here we have Fourier transformed  $\partial_t$  and  $\partial_{x(y)}$  to  $-i\omega$  and  $iq_{x(y)}$  which are the frequency and wavelength of the spin polarized wave. The in plane spin polarization of the TSSs has a very unique property: it is proportional to the charge current perpendicular to it on the TI surface. Therefore the charge current relaxation

time must be equal to the in plane spin relaxation time. A valid spin dynamic equation of the TSSs should be able to reflect this fact. To keep this argument in mind, let us focus on the spin polarization along  $x$ -direction. First we assume that  $\tilde{\Omega} \ll \tilde{\Omega}_{so}$  and  $\tilde{\Delta}_x \ll \tilde{\Omega}_{so}$ . The eigen-frequency of the spin dynamics takes the form

$$i\omega\tau_p = \frac{1 + \tilde{\Delta}_x^2}{2}, \quad (9)$$

which can be Fourier transform to the real space as

$$\partial_t \rho_x = -D_s \partial_x^2 \rho_x - \frac{\rho_x}{2\tau_p}, \quad (10)$$

where  $D_s = v_f^2 \tau_p / 2$ . The prior theory of spin dynamics of the TSSs (Ref.3) is based on the Kubo formula and needs to expand the spin-charge kinetic equation in terms of  $\omega\tau_p$  and  $\tilde{\Delta}_x$  to their leading order. Making the same approximation, our dynamic equation of the spin polarization along  $x$  direction becomes

$$i\omega\tau_p = 1 + \frac{\tilde{\Delta}_x^2}{4} = 0, \quad (11)$$

which is equivalent to

$$\partial_t \rho_x = -\frac{1}{2} D_s \partial_x^2 \rho_x - \frac{\rho_x}{\tau_p}. \quad (12)$$

Eq. (12) is consistent with the spin diffusion equation in Ref. 3 obtained from the linear response theory in the weak SOC limit. However we have found that when  $\omega = 0$ , Eq. (12) gives  $\tilde{\Delta}_x = q^2 l^2 = -4$  which is of the same order but four times larger than the exact solution  $\tilde{\Delta}_x^2 = -1$ . Both  $\tilde{\Delta}_x = -4$  or  $\tilde{\Delta}_x = -1$  are inconsistent with the assumption that  $|\tilde{\Delta}_x| \ll 1$ . On the other hand, the non-perturbative result of Eq. 10 indicates the spin relaxation time is  $\tau_s = 2\tau_p$ , instead of  $\tau_s = \tau_p$  indicated by Eq. 12 based on the perturbative calculation. It is well known that charge transport time  $\tau_{tr}$  for steady current in the system with Dirac-like Hamiltonian is double of the momentum scattering time  $\tau_p$  due to the spin-momentum locked states<sup>4</sup>. Therefore, our non-perturbative theory systematically proves that the spin relaxation time and charge transport time  $\tau_{tr}$  are equal for the TSSs,  $\tau_s = \tau_{tr}$ . This conclusion is consistent with one of the unique properties of the Dirac-like Hamiltonian, that the spin operator is proportional to the velocity operator.

In the case of uniform in plane spin polarization, without assuming  $\tilde{\Omega} \ll \tilde{\Omega}_{so}$ , there is another solution of Eq. A16

$$i\omega\tau_p = \frac{3}{4} \pm i\tilde{\Omega}_{so}, \quad (13)$$

which gives a damped oscillatory spin dynamic mode. Due to the strong SOC, this spin oscillation is accompanied by an AC current with the same frequency. This AC current may provide another way to detect the transport property of TSSs.

*Out of plane spin dynamics.*- next we focus on the spin polarization perpendicular to the surface. The dynamic

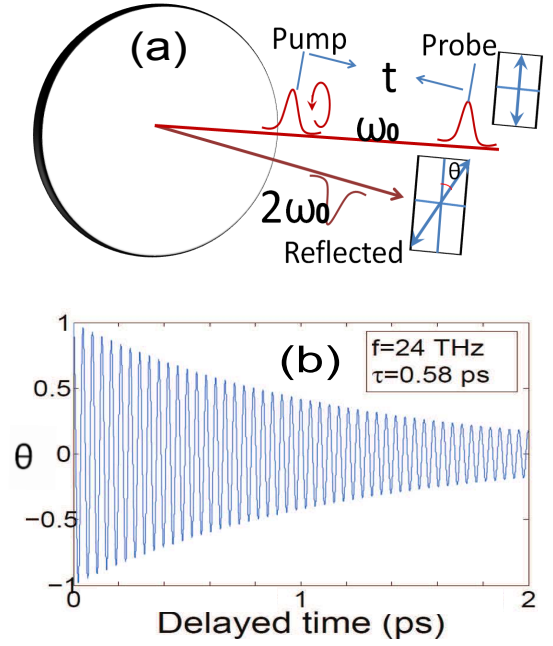


FIG. 2. (a) The second harmonic pumping probe measurement is proposed to observe the dynamics of the out-of-plane spin polarization. The circularized pump light with the frequency  $\omega_0$  is followed by the linear polarized probe light with the same frequency. The time delay is  $t$ . The linear polarized reflected light will only contain the information of the surface states<sup>8</sup>.  $\theta$  is the rotation angle of the linear polarization due to the Kerr effect. (b) The evolution of the uniform out of plane spin polarization. According to our theory, take the experimental parameters from the sample Q2 in table 1 of the Ref.<sup>6</sup> as  $k_f = 0.032 \text{ \AA}^{-1}$ ,  $E_f = 84 \text{ meV}$  and  $k_f l = 69$ .

equation of the spin polarization along  $z$  direction takes the form From Eq. (A16)

$$1 - \frac{\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2}}{\sqrt{\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2} \sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \tilde{\Omega}_{so}^2}} = 0. \quad (14)$$

When  $\omega_z = 0$  for the steady spin polarization, we have

$$\tilde{\Delta}_x = i\sqrt{2 + \tilde{\Omega}_{so}^2} \approx 2k_f l, \quad (15)$$

which means the diffusive length of out of plane spin is of the same order as the Fermi wave length. This is in contrast to the diffusive length in other materials such as the GaAs/AlGaAs where it is of the same order of (or much smaller) than the mean free path  $l$  in the strong (weak) SOC regime<sup>15,17,23,24</sup>. When the spin is uniformly polarized perpendicular to the surface, the eigenfrequency has the form

$$i\omega\tau_p = \frac{1}{2}(1 - \sqrt{1 - 4\tilde{\Omega}_{so}^2}) \approx \frac{1}{2} \pm i\tilde{\Omega}_{so}, \quad (16)$$

where the approximation is valid when  $\tilde{\Omega}_{so} \gg 1$ . Eq. 16 indicates that the spin along the  $z$ -direction will oscillate in a damped form with the frequency equal to

$\tilde{\Omega}_{so} = 2vk_f\tau_p$  and the relaxation time given as  $\tau_s = \tau_{tr}$ , which is the same to the decay rate of the in plane spin polarization. This provides a reliable way to measure the charge transport time  $\tau_{tr}$ . Because the spin along  $z$ -direction is not coupled to any other spin and charge density, this oscillation will not induce current oscillation or charge density oscillation. The experiments have been able to freely tune the Fermi surface of TI close to or away from the Dirac point in a wide range<sup>25</sup>. A circular polarized pump beam can generate spin non-equilibrium polarization of TSSs which has been predicted theoretically<sup>26</sup> and verified experimentally<sup>27</sup>. The spin dynamics of the TISS can be detected by the time-resolved second harmonic optical pump-probe measurements. As only TSSs contribute the second harmonic generation<sup>8,9</sup>, this type of measurement can isolate the surface response from the bulk. If the Fermi surface is turned to 84 meV<sup>6</sup> above the Dirac point, the experiment should observe about 24 THz oscillation through the Kerr rotation angle. The femtosecond pump probe spectroscopy can be used to measure this oscillation. At the same time, the decay rate of this spin oscillation is  $\tau_{tr}$  which gives us the charge transport time of the TSSs (Fig.2).

In conclusion, we develop a non-perturbative method to

obtain the generalized spin dynamic equation of the TSSs which is in the strong SOC regime. Based on this equation, we have found the in-plane spin relaxation time of the pure exponential decay mode is exactly equal to the charge transport time which is consistent to the unique property of the Dirac-like spectrum considered, i.e., the charge current is proportional to the in plane spin polarization. This is a key check of the validity of our theory. We also predict two fast oscillatory modes of spin polarization perpendicular and parallel to the surface of a topological insulator, which cannot be obtained from the prior spin diffusion equations, based on perturbative approaches. Therefore the generalized spin diffusion equation is necessary to quantitatively understand the spin dynamics. At last, we have shown how to read the charge transport properties of TSSs from the out of plane spin dynamics which may provide an alternative way to detect the conductance of the TSSs isolated from the bulk contribution.

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- <sup>1</sup> M. Z. Hasan and C. L. Kane, *Rev. Mod. Phys.* **82**, 3045 (2010).
  - <sup>2</sup> X.-L. Qi and S.-C. Zhang, *Rev. Mod. Phys.* **83**, 1057 (2011).
  - <sup>3</sup> A. A. Burkov and D. G. Hawthorn, *Phys. Rev. Lett.* **105**, 066802 (2010).
  - <sup>4</sup> D. Culcer, E. H. Hwang, T. D. Stanescu, and S. Das Sarma, *Phys. Rev. B* **82**, 155457 (2010).
  - <sup>5</sup> J.-H. Gao, J. Yuan, W.-Q. Chen, Y. Zhou, and F.-C. Zhang, *Phys. Rev. Lett.* **106**, 057205 (2011).
  - <sup>6</sup> D.-X. Qu, Y. S. Hor, J. Xiong, R. J. Cava, and N. P. Ong, *Science* **329**, 821 (2010).
  - <sup>7</sup> J. G. Analytis, R. D. McDonald, S. C. Riggs, J.-H. Chu, G. S. Boebinger, and I. R. Fisher, *Nat Phys* **6**, 960 (2010).
  - <sup>8</sup> D. Hsieh, J. W. McIver, D. H. Torchinsky, D. R. Gardner, Y. S. Lee, and N. Gedik, *Phys. Rev. Lett.* **106**, 057401 (2011).
  - <sup>9</sup> D. Hsieh, F. Mahmood, J. W. McIver, D. R. Gardner, Y. S. Lee, and N. Gedik, *Phys. Rev. Lett.* **107**, 077401 (2011).
  - <sup>10</sup> X. Wang, Y. Du, S. Dou, and C. Zhang, *Phys. Rev. Lett.* **108**, 266806 (2012).
  - <sup>11</sup> D. Zhang, A. Richardella, D. W. Rench, S.-Y. Xu, A. Kandala, T. C. Flanagan, H. Beidenkopf, A. L. Yeats, B. B. Buckley, P. V. Klimov, D. D. Awschalom, A. Yazdani, P. Schiffer, M. Z. Hasan, and N. Samarth, *Phys. Rev. B* **86**, 205127 (2012).
  - <sup>12</sup> Z. Li, T. Chen, H. Pan, F. Song, B. Wang, J. Han, Y. Qin, X. Wang, R. Zhang, J. Wan, D. Xing, and G. Wang, *SCIENTIFIC REPORTS* **2** 595 (2012).
  - <sup>13</sup> S. Raghu, S. B. Chung, X.-L. Qi, and S.-C. Zhang, *Phys. Rev. Lett.* **104**, 116401 (2010).
  - <sup>14</sup> W.-K. Tse and A. H. MacDonald, *Phys. Rev. Lett.* **105**, 057401 (2010).
  - <sup>15</sup> A. A. Burkov, A. S. Núñez, and A. H. MacDonald, *Phys. Rev. B* **70**, 155308 (2004).
  - <sup>16</sup> B. A. Bernevig, J. Orenstein, and S.-C. Zhang, *Phys. Rev. Lett.* **97**, 236601 (2006).
  - <sup>17</sup> T. D. Stanescu and V. Galitski, *Phys. Rev. B* **75**, 125307 (2007).
  - <sup>18</sup> E. G. Mishchenko, A. V. Shytov, and B. I. Halperin, *Phys. Rev. Lett.* **93**, 226602 (2004).
  - <sup>19</sup> X. Liu and J. Sinova, *Phys. Rev. B* **86**, 174301 (2012).
  - <sup>20</sup> J. Rammer, *Quantum Field Theory of Non-equilibrium States* (Cambridge University Press, 2007).
  - <sup>21</sup> C. P. Weber, J. Orenstein, B. A. Bernevig, S.-C. Zhang, J. Stephens, and D. D. Awschalom, *Phys. Rev. Lett.* **98**, 076604 (2007).
  - <sup>22</sup> J. D. Koralek, C. P. Weber, J. Orenstein, B. A. Bernevig, S.-C. Zhang, S. Mack, and D. D. Awschalom, *Nature* **458**, 610 (2009).
  - <sup>23</sup> B. A. Bernevig and J. Hu, *Phys. Rev. B* **78**, 245123 (2008).
  - <sup>24</sup> X. Liu, X.-J. Liu, and J. Sinova, *Phys. Rev. B* **84**, 035318 (2011).
  - <sup>25</sup> D. Hsieh, Y. Xia, L. Wray, D. Qian, A. Pal, J. H. Dil, J. Osterwalder, F. Meier, G. Bihlmayer, C. L. Kane, Y. S. Hor, R. J. Cava, and M. Z. Hasan, *Science* **323**, 919 (2009).
  - <sup>26</sup> H.-Z. Lu, W.-Y. Shan, W. Yao, Q. Niu, and S.-Q. Shen, *Phys. Rev. B* **81**, 115407 (2010).
  - <sup>27</sup> S. Li, H. Huang, W. Zhu, W. Wang, K. Chen, D.-x. Yao, Y. Wang, T. Lai, Y. Wu, and F. Gan, *JOURNAL OF APPLIED PHYSICS* **110** (2011), 10.1063/1.3633228.



# SUPPLEMENTARY ON-LINE MATERIAL FOR "READING CHARGE CURRENT FROM SPIN ON THE SURFACE OF TOPOLOGICAL INSULATOR"

In this appendix, we present the detailed calculation of the spin dynamics on the surface of topological insulator(TI) and how the spin polarization is constructed by the non-equilibrium electrons.

## Appendix A: Spin-charge dynamic equation

We assume that the low energy topological surface state(TSS) has the Dirac-like Hamiltonian plus nonmagnetic short range disorder potential<sup>1,2</sup>

$$\hat{H} = v(\mathbf{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + V_0 \Sigma_i \delta(\mathbf{r} - \mathbf{r}_i) \sigma_0, \quad (\text{A1})$$

where  $v$  is the constant velocity,  $\mathbf{z}$  is the unit vector perpendicular to the surface of TI,  $\mathbf{k}$  is the wave vector of the electron, and  $\sigma_0$  is  $2 \times 2$  identical matrix. Here we assume  $\hbar = 1$  and consider only the spin independent scattering. The velocity operator of this type of Hamiltonian has the form

$$\hat{\mathbf{V}} = \frac{\partial \hat{H}}{\partial \mathbf{k}} = v \mathbf{z} \times \boldsymbol{\sigma}, \quad (\text{A2})$$

and is proportional to the in plane spin polarization perpendicular to the velocity direction.

The dynamics of the spin-charge polarization, as a non-equilibrium process, can be naturally described by quantum kinetic equation<sup>20</sup>

$$\begin{aligned} \partial_t \hat{G}^K + \nabla_{\mathbf{R}} \cdot \left[ \frac{1}{2} \{ \hat{\mathbf{V}}_{\mathbf{k}}, \hat{G}^K \} \right] + i[\hat{H}_0(\mathbf{k}), \hat{G}^K] \\ = -i \left[ (\hat{\Sigma}^R \hat{G}^K - \hat{G}^K \hat{\Sigma}^A) - (\hat{G}^R \hat{\Sigma}^K - \hat{\Sigma}^K \hat{G}^A) \right], \end{aligned} \quad (\text{A3})$$

where  $t$  and  $\mathbf{R}$  are time and real space variants,  $\hat{G}^K$  is the  $2 \times 2$  matrix of spin- $\frac{1}{2}$  Keldysh Green's function,  $\hat{\mathbf{V}} = v(\mathbf{z} \times \boldsymbol{\sigma})$  is the velocity operator,  $\hat{H}_0(\mathbf{k}) = v(\mathbf{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k}$  and  $\Sigma^{R(A,K)}$  is the retarded (advanced, Keldysh) self energy due to disorder potential. The term  $[\frac{1}{2} \{ \hat{\mathbf{V}}_{\mathbf{k}}, \hat{G}^K \}] = \hat{\mathbf{J}}$  is natural definition of current matrix. The third term in the Eq. (A3) is the spin torque exerted by the Rashba SOI. In this work, the operator with a hat means it is a matrix. In the equilibrium state, the Keldysh Green's function satisfies<sup>20</sup>

$$\hat{G}_0^K = (\hat{G}^R - \hat{G}^A) \tanh\left(\frac{E - \epsilon_f}{2k_B T}\right), \quad (\text{A4})$$

where  $G_0^K$  stands Keldysh Green's function in equilibrium,  $k_B$  is the Boltzmann constant and  $T$  here is the system temperature. Based on Eq. (A4) and we assume that the Keldysh Green's function generally has the form

$$\hat{G}^K = -2\pi i \delta(E - \epsilon_k^+) \hat{h}^+ - 2\pi i \delta(E - \epsilon_k^-) \hat{h}^-, \quad (\text{A5})$$

where  $\epsilon_k^\pm = \pm v k$ ,  $\hat{h}^\pm(\mathbf{k}, \mathbf{R}, T)$  is the distribution function, defined as

$$\hat{h}(\mathbf{k}, \mathbf{R}, t) = - \int_{-\infty}^{\infty} \frac{dE}{2\pi i} \hat{G}_{\mathbf{k}, E}^K(\mathbf{R}, t) \quad (\text{A6})$$

and  $\pm$  label the distribution function of the electrons spin sub-band above(below) Dirac point. Normally the non-equilibrium distribution function  $\delta \hat{h}$  locate around Fermi energy. Therefore we define the non-equilibrium thermal average distribution function as

$$\hat{g}^\pm(\mathbf{e}_{\mathbf{k}}, \mathbf{R}, t) = \int N(\epsilon_k) d\epsilon_k \delta \hat{h}^\pm(\mathbf{k}, \mathbf{R}, T) \quad (\text{A7})$$

where  $\mathbf{e}_{\mathbf{k}} = \mathbf{k}/k$  is the unit vector along  $\mathbf{k}$  direction and  $N(\epsilon_k) = k/hv$  is the density of state. In this work, we consider the case that the Fermi energy is above the Dirac point and much larger than  $k_B T$ .

To obtain the kinetic equation of distribution function, we introduce the non-equilibrium density matrix<sup>19</sup>

$$\hat{\rho}(\mathbf{R}, t) = \frac{i}{2\pi N(\epsilon_k)} \int \frac{d^2 k}{(2\pi)^2} \delta \hat{h} = \int \frac{d\theta}{2\pi} \delta \hat{g}(\mathbf{k}_{\mathbf{f}}, \mathbf{R}, t), \quad (\text{A8})$$

where  $\theta$  is the angel between  $\mathbf{k}_f$  and  $x$  axis. By integrating out energy  $E$  and  $\epsilon_k$  The Eq. A3 can be converted to

$$\partial_t \hat{g} + \nabla_{\mathbf{R}} \cdot \left\{ \frac{1}{2} \hat{\mathbf{V}}, \hat{g} \right\} + i[\hat{H}(\mathbf{k}_f), \hat{g}] + \frac{\hat{g}}{\tau_p} = \frac{\hat{\rho}(\mathbf{R}, T)}{\tau_p}. \quad (\text{A9})$$

where

$$1/\tau_p = \frac{\pi n_i V_0^2}{\hbar} N(\epsilon_{k_f})$$

is the momentum scattering time at Fermi surface and  $n_i$  is the 2D density of the nonmagnetic impurities.

The non-equilibrium thermal average distribution function and density matrix can be generally written as

$$\begin{aligned} \hat{g} &= g_c \sigma_0 + g_x \sigma_x + g_y \sigma_y + g_z \sigma_z, \\ \hat{\rho} &= \rho_c \sigma_0 + \rho_x \sigma_x + \rho_y \sigma_y + \rho_z \sigma_z. \end{aligned} \quad (\text{A10})$$

If we multiply  $\sigma_i$  where  $i = 0, x, y, z$  on both sides of Eq. A3 and calculate the trace, using the fact that  $\text{Tr}(\sigma_i \sigma_j)/2 = \delta_{ij}$ , the quantum kinetic equation can be written in the classical spin-charge 4D space after integrating out  $E$  as<sup>19</sup>

$$\hat{K} \begin{pmatrix} g_0 \\ g_x \\ g_y \\ g_z \end{pmatrix} = i \begin{pmatrix} \rho_0 \\ \rho_x \\ \rho_y \\ \rho_z \end{pmatrix}, \quad (\text{A11})$$

where

$$\hat{K} = \begin{pmatrix} \tilde{\Omega} & -i\tilde{\Delta}_y & i\tilde{\Delta}_x & 0 \\ -i\tilde{\Delta}_y & \tilde{\Omega} & 0 & -\tilde{\Omega}_{so} \cos(\theta) \\ i\tilde{\Delta}_x & 0 & \tilde{\Omega} & -\tilde{\Omega}_{so} \sin(\theta) \\ 0 & \tilde{\Omega}_{so} \cos(\theta) & \tilde{\Omega}_{so} \sin(\theta) & \tilde{\Omega} \end{pmatrix}, \quad (\text{A12})$$

$\tilde{\Omega} = 1 - i\omega\tau_p$ ,  $\tilde{\Omega}_{so} = 2vk_f\tau_p$  and  $\tilde{\Delta}_{x(y)} = lq_{x(y)}$  is from the anti-commutator on the left hand side of Eq. (A9) which gives the spin-charge coupling. Here we have Fourier transformed  $\partial_t$  and  $\partial_{x(y)}$  to  $-i\omega$  and  $iq_{x(y)}$  which are the frequency and wavelength of the spin polarized wave. For convenience, in the rest of this paper we will express frequency in units of  $1/\tau_p$  and wave vector in units of  $1/l$ , unless otherwise stated. The difficulty of obtaining the spin dynamics equation in the strong SOC regime lies on the fact that the three terms, spin precession angle  $2vk_f\tau_p$ , the dimensionless time and spacial spin relaxation rate  $\omega\tau_p$  and  $ql$ , may be large simultaneously and cannot be treated perturbatively. Here, we abandon the idea of gradient expansion in terms of  $\omega\tau_p$  and  $ql$  and derive the spin-charge diffusion equation by simply multiplying  $K^{-1}$  on both sides of Eq. (A11) and integrating out the angle  $\theta$ . To simplify our discussion, we consider the spin wave vector is only along  $x$  direction and takes  $q_y = 0$ . In this case, using the relation Eq. (A11) the spin-charge dynamic equation of the density coefficient  $\rho_{c(x,y,z)}$  can be obtained as

$$-i \int \frac{d\theta}{2\pi} \begin{pmatrix} g_0 \\ g_x \\ g_y \\ g_z \end{pmatrix} = \begin{pmatrix} \rho_0 \\ \rho_x \\ \rho_y \\ \rho_z \end{pmatrix} = \hat{D} \begin{pmatrix} \rho_0 \\ \rho_x \\ \rho_y \\ \rho_z \end{pmatrix}, \quad (\text{A13})$$

where  $\hat{D} = \int \frac{d\theta}{2\pi} \hat{K}^{-1}$  and  $\hat{K}^{-1}$  takes the form

$$\begin{pmatrix} \tilde{\Omega} (\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2) & i \cos(\theta) \sin(\theta) \tilde{\Delta}_x \tilde{\Omega}_{so}^2 & -i \tilde{\Delta}_x (\tilde{\Omega}^2 + \cos^2(\theta) \tilde{\Omega}_{so}^2) & -i \tilde{\Omega} \sin(\theta) \tilde{\Delta}_x \tilde{\Omega}_{so} \\ i \cos(\theta) \sin(\theta) \tilde{\Delta}_x \tilde{\Omega}_{so}^2 & \tilde{\Omega} (\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \sin^2(\theta) \tilde{\Omega}_{so}^2) & -\tilde{\Omega} \cos(\theta) \sin(\theta) \tilde{\Omega}_{so}^2 & \cos(\theta) (\tilde{\Omega}^2 + \tilde{\Delta}_x^2) \tilde{\Omega}_{so} \\ -i \tilde{\Delta}_x (\tilde{\Omega}^2 + \cos^2(\theta) \tilde{\Omega}_{so}^2) & -\tilde{\Omega} \cos(\theta) \sin(\theta) \tilde{\Omega}_{so}^2 & \tilde{\Omega}^3 + \cos^2(\theta) \tilde{\Omega}_{so}^2 \tilde{\Omega} & \tilde{\Omega}^2 \sin(\theta) \tilde{\Omega}_{so} \\ i \tilde{\Omega} \sin(\theta) \tilde{\Delta}_x \tilde{\Omega}_{so} & -\cos(\theta) (\tilde{\Omega}^2 + \tilde{\Delta}_x^2) \tilde{\Omega}_{so} & -\tilde{\Omega}^2 \sin(\theta) \tilde{\Omega}_{so} & \tilde{\Omega} (\tilde{\Omega}^2 + \tilde{\Delta}_x^2) \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_x \\ \rho_y \\ \rho_z \end{pmatrix} \quad (\text{A14})$$

The Eq. (A13) is a generalized spin diffusion equation and valid from the weak to the strong SOC regime. It is noted that the denominator of  $K^{-1}$  is the function of  $\cos^2(\theta)$ . By using the property of trigonometric functions without

calculating the integral of  $\theta$ , it can be easily proved that the spin polarization along  $x$  and  $z$  direction is not coupled to other components. Therefore the Eq. (A13) can be block diagonalized as

$$\begin{pmatrix} 1 - \frac{\tilde{\Omega}(\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2)}{\tilde{\Omega}\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2}\sqrt{\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2}\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \tilde{\Omega}_{so}^2}} & i\left(\frac{1}{\tilde{\Delta}_x} - \frac{\tilde{\Omega}\sqrt{\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2}}{\tilde{\Delta}_x\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2}\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \tilde{\Omega}_{so}^2}}\right) \\ i\left(\frac{1}{\tilde{\Delta}_x} - \frac{\tilde{\Omega}\sqrt{\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2}}{\tilde{\Delta}_x\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2}\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \tilde{\Omega}_{so}^2}}\right) & 1 - \tilde{\Omega}\left(\frac{1}{\tilde{\Delta}_x^2} - \frac{\tilde{\Omega}\sqrt{\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2}}{\tilde{\Delta}_x^2\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2}\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \tilde{\Omega}_{so}^2}}\right) \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_y \end{pmatrix} = 0 \quad (\text{A15})$$

$$\begin{pmatrix} 1 - \left(\frac{\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2}\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \tilde{\Omega}_{so}^2}}{\tilde{\Delta}_x^2\sqrt{\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2}} - \frac{\tilde{\Omega}}{\tilde{\Delta}_x^2}\right) & 0 \\ 0 & 1 - \frac{\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2}}{\sqrt{\tilde{\Omega}^2 + \tilde{\Omega}_{so}^2}\sqrt{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \tilde{\Omega}_{so}^2}} \end{pmatrix} \begin{pmatrix} \rho_x \\ \rho_z \end{pmatrix} = 0 \quad (\text{A16})$$

For the spin-charged coupled equation, Eq. A15, when the spin is uniformly polarized, say  $\tilde{\Delta}_x = 0$ , the off diagonal terms in the spin dynamic matrix vanish. Therefore, the charge and spin densities for the uniform polarization are independent.

### Appendix B: In-plane spin dynamics under diffusive approximation

Now, let us focus on the in-plane spin polarization along  $x$  direction. It has been proved exactly to not couple the spin polarization in other directions. Therefore we only need to calculate the element  $\hat{D}_{22}$  which takes the form

$$\hat{D}_{22} = \int \frac{d\theta}{2\pi} \frac{-\sin^2 \theta \cos \theta \tilde{\Delta}_x \tilde{\Omega}_{so}^2 + \tilde{\Omega} \left( \tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \sin^2(\theta) \tilde{\Omega}_{so}^2 \right)}{\left( \tilde{\Omega}^2 + \tilde{\Omega}_{so}^2 \right) \tilde{\Omega}^2 + \tilde{\Delta}_x^2 \left( \tilde{\Omega}^2 + \cos^2(\theta) \tilde{\Omega}_{so}^2 \right)}, \quad (\text{B1})$$

Due to the fact that  $\sin^2(\theta + \pi) \cos(\theta + \pi) = -\sin^2 \theta \cos \theta$ , we can drop the first term in the integrated function of Eq. B1 and have

$$\hat{D}_{22} = \int \frac{d\theta}{2\pi} \frac{\tilde{\Omega} \left( \tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \sin^2(\theta) \tilde{\Omega}_{so}^2 \right)}{\left( \tilde{\Omega}^2 + \tilde{\Omega}_{so}^2 \right) \tilde{\Omega}^2 + \tilde{\Delta}_x^2 \left( \tilde{\Omega}^2 + \cos^2(\theta) \tilde{\Omega}_{so}^2 \right)}. \quad (\text{B2})$$

Taking the diffusive approximation  $\tilde{\Delta}_x \ll 1$  and  $\omega\tau_p \ll 1$  while  $\tilde{\Omega}_{so} \gg 1$ , we expand the Eq. B2 up to the first nonzero order in terms of  $\tilde{\Delta}_x$  and  $\tilde{\Omega}_{so}$  as

$$\begin{aligned} \hat{D}_{22} &= \int \frac{d\theta}{2\pi} \frac{\tilde{\Omega} \left( \tilde{\Omega}^2 + \tilde{\Delta}_x^2 + \sin^2(\theta) \tilde{\Omega}_{so}^2 \right)}{\left( \tilde{\Omega}^2 + \tilde{\Omega}_{so}^2 \right) \tilde{\Omega}^2 + \tilde{\Delta}_x^2 \left( \tilde{\Omega}^2 + \cos^2(\theta) \tilde{\Omega}_{so}^2 \right)} \\ &\approx \int \frac{d\theta}{2\pi} \frac{\tilde{\Omega} \sin^2 \theta}{\tilde{\Omega}^2 + \tilde{\Delta}_x^2 \cos^2 \theta} \approx \frac{1}{2} (1 + i\omega\tau - \frac{\tilde{\Delta}_x^2}{2}). \end{aligned} \quad (\text{B3})$$

Substituting Eq. B3 to the generalized spin dynamic equation Eq. A13, we have

$$i\omega\tau_p = 1 + \frac{1}{2} \tilde{\Delta}_x^2, \quad (\text{B4})$$

which can be Fourier transformed to the real space as

$$\partial_t \rho_x = -D_s \partial_x^2 \rho_x - \frac{\rho_x}{2\tau_p}, \quad (\text{B5})$$

where  $D_s = v_f^2 \tau_p / 2$ . This is equivalent to the in-plane spin diffusive equation in Ref.3. (Here we assuming spin wave vector along  $x$  direction and the term contain  $\partial_y$  is zero).

### Appendix C: The spin polarization texture in 2DEG and on the surface of TI

In this section, we intuitively show why spin helix mode is absent on the surface of TI. In the following derivation, we focus on the  $k_y = 0$  channel to simple our calculation.

The spin wave operator in real space is defined as

$$\hat{S}_+(x) = \sum_k \left( C_{k+q,\uparrow}^\dagger C_{k,\downarrow} \frac{e^{-iqx}}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} + C_{k,\downarrow}^\dagger C_{k+q,\uparrow} \frac{e^{iqx}}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \right) \quad (C1)$$

and

$$\hat{S}_-(x) = \sum_k \left( C_{k-q,\uparrow}^\dagger C_{k,\downarrow} \frac{e^{iqx}}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} + C_{k,\downarrow}^\dagger C_{k-q,\uparrow} \frac{e^{-iqx}}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \right) \quad (C2)$$

First, let us consider the spin polarization on the 2DEG. The operator  $\hat{S}_+$  actin on electron states gets an spin density wave which has the form

$$\begin{aligned} S_+(x) = \hat{S}_+|\psi\rangle &= \sum_k \left( \sqrt{h_{k,\downarrow}(1-h_{k+q,\uparrow})} \frac{e^{-iqx}}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} \right. \\ &\quad \left. + \sum_k \left( \sqrt{h_{k+q,\uparrow}(1-h_{k,\downarrow})} \frac{e^{iqx}}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \right) \right) \\ &= \sum_k \sqrt{h_k(1-h_k)} (\cos(qx)\sigma_z - \sin(qx)\sigma_x). \end{aligned} \quad (C3)$$

where  $h_{k,\uparrow(\downarrow)}$  is occupied probability which is the diagonal element of the distribution function in Eq. A6. Here, in the case of  $q \ll k_f$ , we make an approximation that  $h_{k+q,\uparrow} = h_{k,\downarrow}$ . The spin polarization given by Eq. C3 in three directions are  $\langle S_z \rangle = \cos(qx)$ ,  $\langle S_x \rangle = -\sin(qx)$  and  $\langle S_y \rangle = 0$  which is a contour-clock wise spin helix mode in  $x - z$  plane.

Similar the clockwise spin helix mode is constructed by

$$\begin{aligned} S_-(x) = \langle \hat{S}_-(x) \rangle &= \sum_k \left( \sqrt{f_{k-q,\uparrow}f_{k,\downarrow}(1-f_{k-q,\uparrow})(1-f_{k,\downarrow})} \frac{e^{iqx}}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} \right. \\ &\quad \left. + \sum_k \left( \sqrt{f_{k-q,\uparrow}f_{k,\downarrow}(1-f_{k-q,\uparrow})(1-f_{k,\downarrow})} \frac{e^{-iqx}}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \right) \right) \\ &\approx \sum_k \sqrt{h_k(1-h_k)} (\cos(qx)\sigma_z + \sin(qx)\sigma_x), \end{aligned} \quad (C4)$$

whose spin polarization in three directions are  $\langle S_z \rangle = \cos(qx)$ ,  $\langle S_x \rangle = \sin(qx)$  and  $\langle S_y \rangle = 0$ .

On the surface of TI, there is only one spin-sub band at the Fermi surface. The other sub-band is below the Dirac point and thereby far below the Fermi energy in the condition  $E_f \gg kT$ . Accordingly, for the counter-clockwise spin helix mode in Eq. C3,  $h_{k+q,\uparrow}$  and  $h_{k,\downarrow}$  can not be approximately equal because they belong to different spin-sub band and has the energy difference about  $2E_f$ . For example, when  $k < 0$ , as shown in Fig.1b in the paper, the state  $|k+q, \uparrow\rangle$  is below the Dirac point and completely occupied so that  $h_{k+q<0,\downarrow} = 1$ . Similar we also have  $h_{k>0,\uparrow} = 1$ . As a result, the terms containing  $\sum_{k>0} C_{k,\downarrow}^\dagger C_{k+q,\uparrow}$  ( $\sum_{k+q<0} C_{k+q,\uparrow}^\dagger C_{k,\downarrow}$ ) becomes zero because they are proportional to  $\sqrt{1-h_{k+q<0,\uparrow}} = 0$  ( $\sqrt{1-h_{k>0,\downarrow}} = 0$ ). This implies hat only half terms in Eq. C3 which have the form

$$\begin{aligned} S_+^{\text{half}} &= \sum_{k+q>0} \langle C_{k+q,\uparrow}^\dagger C_{k,\downarrow} \rangle + \sum_{k<0} \langle C_{k,\downarrow}^\dagger C_{k+q,\uparrow} \rangle \\ &= \sum_{k+q>0} \sqrt{1-h_{k+q,\uparrow}} \frac{e^{-iqx}}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} + \sum_{k<0} \sqrt{1-h_{k,\downarrow}} \frac{e^{iqx}}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \end{aligned} \quad (C5)$$

will contribute to the spin polarization. Similar, for the clockwise spin helix mode, only half terms in Eq. C4 which have the form

$$\begin{aligned} S_-^{\text{half}} &= \sum_{k-q>0} \langle C_{k-q,\uparrow}^\dagger C_{k,\downarrow} \rangle + \sum_{k<0} \langle C_{k,\downarrow}^\dagger C_{k-q,\uparrow} \rangle \\ &= \sum_{k-q>0} \sqrt{1-h_{k-q,\uparrow}} \frac{e^{iqx}}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} + \sum_{k<0} \sqrt{1-h_{k,\downarrow}} \frac{e^{-iqx}}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \end{aligned} \quad (C6)$$



will contribute to the spin polarization. By redefining  $k + q \rightarrow k$  and  $k - q \rightarrow k$  in Eq. C5 and Eq. C6 separately, we obtain the spin polarization on the surface as

$$\begin{aligned}
 S &= S_+^{\text{half}} + S_-^{\text{half}} = \sum_{k>0} \sqrt{1-h_{k,\uparrow}} \frac{e^{-iqx}}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} + \sum_{k<0} \sqrt{1-h_{k,\downarrow}} \frac{e^{iqx}}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \\
 &\quad + \sum_{k>0} \sqrt{1-h_{k,\uparrow}} \frac{e^{iqx}}{2} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} + \sum_{k<0} \sqrt{1-h_{k,\downarrow}} \frac{e^{-iqx}}{2} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \\
 &= \sum_{k>0} \sqrt{1-h_{k,\uparrow}} \cos(qx) \sigma_z + \sum_{k<0} \sqrt{1-h_{k,\downarrow}} \cos(qx) \sigma_z = \sum_k \sqrt{1-h_k^+} \cos(qx) \sigma_z, \quad (\text{C7})
 \end{aligned}$$

where  $h_k^+$  is the distribution of the spin-sub band above Dirac point and defined in Eq. A5 and Eq. A6 which only has finite spin polarization along  $z$  direction and will not couple to  $x$  direction.

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